1,1,2,2-Tetrahydroperfluoro-1-decanol

678-39-7 | DTXSID7029904

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 8.03e-15 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.10e-01

Confidence level: 4.85e-01

Nearest Neighbors from the Training Set

Image not found
Butane, 1,1,1,2,2,3,3,4,4-
nonafluoro-4-methoxy-
Measured: 7.20e-15
Predicted: 1.32e-14

Image not found
Perfluorotributylamine
Measured: 6.00e-17
Predicted: 1.14e-16

Image not found
1-Butanol, 2,2,3,3,4,4,4-
heptafluoro-
Measured: 1.12e-13
Predicted: 6.54e-14

Image not found
HFE-347pcf2
Measured: 9.40e-14
Predicted: 6.55e-14

Image not found
Propane, 1,1,1,2,2,3,3-
heptafluoro-3-methoxy-
Measured: 1.18e-14
Predicted: 1.85e-14